

Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

February 10, 2017

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Applications Team Characterizes I/O Performance of New Electra Supercomputer



- HECC's Application Performance and Productivity (APP) team conducted extensive testing of I/O performance on the new Electra supercomputer.
- Electra is housed in the Modular Supercomputing Facility (MSF) adjacent to Bldg. N258, and has no user filesystems co-located with it. Instead, it connects to filesystems n
- In the main facility via a network that uses MetroX InfiniBand extenders and Lustre routers.
- The uniqueness of this setup necessitated extensive testing to ensure that application I/O performance would be similar to what users experience on Pleiades.
 - The APP team investigated the sensitivity of I/O performance to the number of Lustre routers used to connect to the filesystems.
 - They found that using 10 Lustre routers for Electra provided equivalent performance to jobs running on Pleiades.
- Future expansion of the MSF can be accommodated over the existing infrastructure, potentially adding additional MetroX links and Lustre routers if needed.

Mission Impact: Extensive testing to evaluate I/O performance reduces risks associated with the new deployment and enables HECC to provide better advice to users seeking to optimize code performance.



Electra supercomputer users get access to their files in the main facility via Mellanox MetroX MTX6000 InfiniBand extenders, which connect the Electra fabric in the Modular Supercomputing Facility to Lustre routers on the InfiniBand fabric in the NAS facility over 16 fiber optic links, each about 1,000 feet long.

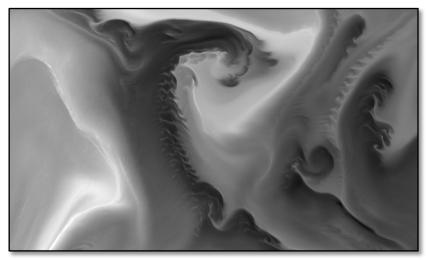
POCs: Henry Jin, haoqiang.jin@nasa.gov, NASA Advanced Supercomputing (NAS) Division; Robert Hood, robert.hood@nasa.gov, NAS Division, CSRA LCC

Highly Parallel Input/Output Routines in MITgcm Demonstrate MSF Capabilities



- HECC visualization experts developed highly parallel input/output routines to enable extremely highresolution ocean modeling runs on 30,000 cores of Electra, accessing filesystems on Pleiades' network, using the high-end MIT General Circulation Model (MITgcm) employed by the Estimating the Circulation and Climate of the Ocean (ECCO) project team.
- Newly developed input routines, using industrystandard MPI-IO, cut model startup times from hours to minutes.
 - 1.5 terabytes (TB) of input data was read and distributed across 30,000 compute ranks in less than 5 minutes.
- Custom output routines, developed from the Visualization team's concurrent visualization framework, enabled filesystem writes at hardware speeds.
 - Combined diagnostic and checkpoint output of greater than 2 TB was written in less than 2 minutes, with peak rates of ~45 gigabytes per second (GB/s).
- The team used the high-bandwidth MITgcm application to stress-test the network connections between Electra and the Pleiades filesystems.
- MITgcm application was able to take full advantage of the newly deployed Electra/Pleiades capabilities to enable scientifically useful computations at unprecedented detail and resolution.

Mission Impact: HECC's extreme-scale deployment of a highly optimized code confirmed the excellent performance and utility of the MSF installation, and enabled new science with a community-standard model run at unprecedented resolution.



Tiny piece of a computational domain shows swirling temperature variations at 250 meters/pixel just outside San Francisco Bay. *Chris Henze. NASA/Ames*

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HECC Implements Cost-Effective Expansion of Merope Supercomputer



- HECC engineers completed an expansion of the Merope supercomputer with 640 additional Westmere nodes. This represents a 55% increase in computing capacity on Merope.
- The expansion comprises repurposed
 Westmere nodes retired from Pleiades to
 provide the power and cooling necessary for
 the Broadwell augmentation to Pleiades.
- The nodes were integrated into Merope during a system maintenance downtime. Due to floor-load constraints, the nodes are housed in 20 half-populated racks.
- In addition to providing computational resources to HECC users, the Merope cluster serves as a platform for large-scale system tests that could adversely impact users on Pleiades.

Mission Impact: Repurposing retired hardware enables HECC to cost-effectively deliver additional computational cycles to NASA users.



Twenty half-populated racks were installed in the Merope supercomputer, located at the secondary compute facility at NASA Ames. The racks are half populated due to floor-load constraints.

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HECC Account Request System Enhanced to Improve RSA Token Renewal Requests



- The HECC Tools team enhanced the Account Request System to include the capability for users to renew their expiring RSA tokens online, eliminating the need for staff to manually contact users for upcoming renewals. The HECC Accounts team now send users with expiring tokens the Account Request System link to renew their tokens.
- Development of the token renewal feature included:
 - Parsing the RSA token information from the Radius database.
 - Developing options to allow users to select soft tokens (iOS or Android) or token fobs.
 - Obtaining correctly formatted mailing addresses for hard tokens and providing detailed emails and instructions for setting up the multiple steps necessary for soft tokens.
- Future plans include developing a screencast for the soft token setup, and automating user notifications based on the token expiration date.

Mission Impact: Online renewal of NASA's required two-factor authentication RSA tokens provides a streamlined workflow for ensuring that token renewals are efficiently handled for HECC users.



Screenshot of the updated Account Request System that allows users to request either soft tokens or physical fobs to replace their expiring RSA tokens for two-factor authentication to log into HECC systems.

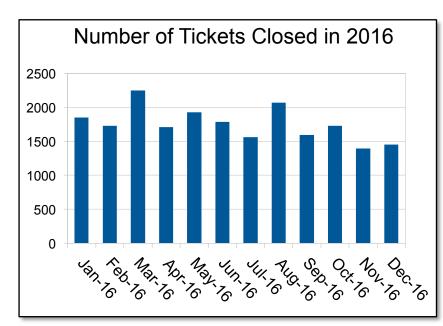
POC: Ryan Spaulding, ryan.c.spaulding@nasa.gov, (408) 772-6567, NASA Supercomputing Division, ADNET Systems

HECC Support Staff Continue Providing Excellent Help to Users



- In 2016, HECC staff provided support to more than a thousand users from all of NASA's mission directorates.
- Support staff across the HECC project processed, tracked, and resolved over 21,000 tickets for the 12 months from January 1, 2016 through December 31, 2016.
- Tickets covered a wide range of support activities—from automated notifications of system issues to resolving a variety of issues for users calling for help:
 - Answered inquiries about accounts, failed jobs, and status of systems.
 - Extended run-times of already-queued or running jobs.
 - Modified allocations and account expiration dates.
 - Explained file transfer tools and processes.
 - Debugged job failures and identifying execution bottlenecks.

Mission Impact: The 24x7 support services provided by HECC experts resolve system problems and users' technical issues, and enable users to focus on their critical mission projects.



HECC staff typically resolved just under 1,800 Remedy tickets per month in 2016—just over 21,000 tickets total.

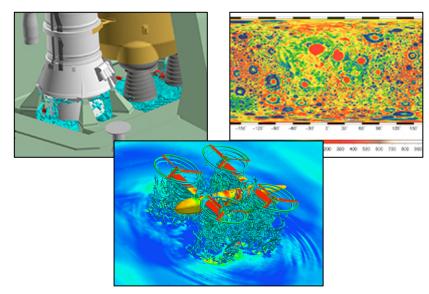
POC: Leigh Ann Tanner, leighann.tanner@nasa.gov, (650) 604-4468, NASA Advanced Supercomputing Division, CSRA LLC

January 2017 HECC Supercomputer Usage Sets New High of 22.76 Million SBUs



- In January, combined usage on HECC supercomputers set a new record.
- 22,757,811 Standard Billing Units (SBUs*)
 were used on Pleiades, Electra, Merope, and
 Endeavour by NASA's science and
 engineering organizations.
- Usage exceeded by about half a million SBUs the previous record of 22.3 million set in December 2016.
- This increase was enabled by the addition of Electra and the expansion of Merope.
- Over 310 projects from all across NASA used time on one or more HECC systems.
- The top 10 projects used from 459,306 to 3,188,080 SBUs each and together accounted for over 43% of total usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA's users.

Mission Impact: Increasing capacity of HECC systems provides Mission Directorates with more resources for the accomplishment of their goals and objectives.



Images representing computing projects from different Mission Directorates. From top left: (1) Image from a simulation of the Ignition Over-Pressure system projecting water during ignition. *Jeff West, NASA/Marshall.* (2) Map of the gravity field of the moon as measured by NASA's Gravity Recovery and Interior Laboratory mission. *NASA/JPL-Caltech; NASA/Goddard; MIT.* (3) Visualization of NASA's conceptual design of a large-scale quadrotor vehicle. *S. Yoon, NASA/Ames.*

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

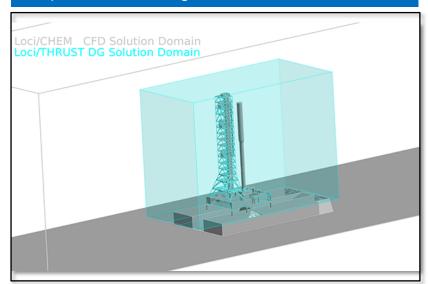
^{* 1} SBU equals 1 hour of a Pleiades Westmere 12-core node.

Improving Fidelity of Launch Vehicle Liftoff Acoustic Simulations *



- Researchers at Marshall Space Flight Center (MSFC) used a hybrid CFD and computational aero-acoustics (CFD/CAA) modeling framework to simulate highly complex plume formation and interaction with launch pad geometry to accurately model the reflection and refraction of acoustic waves on launch pad components.
- The MSFC team's CFD/CAA code was developed to improve such liftoff acoustic environment predictions and optimized for running on Pleiades.
 - The new CFD/CAA approach proved highly capable of accurately propagating and conserving the acoustic wave field over the complex launch vehicle and launch pad geometry.
 - Numerical simulations can be applied in evaluating various sound suppression measures, reducing the need for expensive testing.
- HECC supercomputing resources are instrumental in completing this type of analysis. The model requires ~300 million mesh cells to simultaneously resolve the launch vehicle and launch pad details and adequately capture the acoustic sources at the rocket plumes.

Mission Impact: Enabled by the Pleiades supercomputer, the improved capability to perform high-fidelity computational acoustic field simulations will increase confidence in the characterization of launch acoustic loads environments through computational modeling.



The Loci/THRUST acoustic solver domain is embedded in the Loci/CHEM CFD simulation domain. Acoustic wave input is received through boundary patches located near the acoustic source regions, such as near the flame trench under the launch platform, the top of the flame trench, and inside the launch mount.

POCs: Peter Liever, peter.a.liever@nasa.gov, (256) 544.3288, Jeff West, jeffrey.s.west@nasa.gov, (256) 544.6309, NASA Marshall Space Flight Center

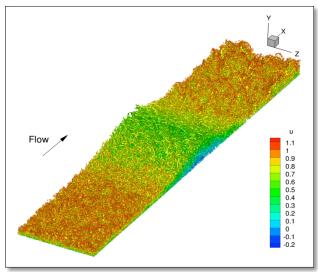
^{*} HECC provided supercomputing resources and services in support of this work

Running Simulations on Pleiades to Improve Engineering Models for Aerospace Design *



- Predicting the behavior of turbulent flow passing over an aircraft or spacecraft is one of the most important tasks involved in designing such vehicles. It is also one of the most difficult.
- To improve engineering turbulence models, researchers at NASA Langley are running turbulent flow simulations on Pleiades to obtain high-fidelity benchmark data needed for more accurate models.
 - A family of cases was obtained by computing the equations governing the flow over a smooth flat surface, under conditions representative of air passing over a flight vehicle.
 - Conditions were adjusted to produce separation of the turbulent boundary layer (air adjacent to the surface), enabling the analysis of one of the most important and difficult-to-model features of an aerodynamic flow.
- Results are being used to quantify the shortcomings of current turbulence models and identify improvements required for next-generation models.
- These improvements could lead to superior vehicle design, in terms of flight characteristics and fuel efficiency, as well as lower the risk and cost of future aircraft and space vehicles.

Mission Impact: Run on HECC resources, these simulations support the Transformational Tools & Technologies Project of NASA's Transformative Aeronautics Concepts Program, helping to develop computational tools to design aerospace vehicles.



Simulation of separated, turbulent, swept-wing boundary layer, run on Pleiades. Turbulence structures are represented by isocontours of Q-criteria, colored by chordwise velocity u. Note the separation and reattachment of the turbulence from/to the bottom surface. This type of flow, common in aerospace applications, is one of the most important and difficult features to account for in the design of air- and spacecraft.

POCs: Gary Coleman, gary.n.coleman@nasa.gov, (757) 864-5486, Christopher Rumsey, c.l.rumsey@nasa.gov, (757) 864-2165, NASA Langley Research Center

^{*} HECC provided supercomputing resources and services in support of this work.

HECC Facility Hosts Several Visitors and Tours in January 2017



- HECC hosted 11 tour groups in January; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Visitors this month included:
 - Meg Whitman, President and Chief Executive Officer of Hewlett Packard Enterprise, and several members of her team, were briefed by Ames executive management and visited the NAS facility.
 - Mike Mastaler, Director of the NASA Space Environments
 Testing Management Office (STEMO) received Ames
 executive management reviews and a Center tour that
 included the HECC Modular Supercomputing Facility.
 - David Horner, Director, Department of Defense (DoD), High Performance Computing Modernization Program (HPCMP), and Sandy Landsberg, Deputy Director, DoD HPCMP, had discussions with HECC/NAS management about HPC at NASA to explore areas of mutual interest.
 - David Hazlehurst, Australia's Deputy Secretary for Industry, Innovation & Science and a group from that office received a executive management review that included the NAS Facility.
 - Mark Glorioso, Director, NASA Shared Services Center.
 - Andy Schain, Data Integration Integrated Task Team lead for the Exploration Systems Division.
 - 20 new civil servants hired at Ames.



HECC Deputy Project Manager William Thigpen gives an overview of the Pleiades supercomputer and NAS facility capabilities to Hewlett Packard Enterprise President and Chief Executive Officer, Meg Whitman, and team.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers



- "What is the Maximum Mass of a Population III Galaxy?" E. Visbal, G. Bryan,
 Z. Haiman, arXiv:1701.00814 [astro-ph.GA], January 3, 2017. *
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- "In-Situ GPS Records of Surface Mass Balance and Ocean-Induced Basal Melt for Pine Island Glacier, Antarctica," D. Shean, et al., The Cryosphere: Discussions, January 3, 2017. *
 - http://www.the-cryosphere-discuss.net/tc-2016-288/tc-2016-288.pdf
- "Coronal Jets Simulated with the Global Alfvén Wave Solar Model," J. Szente, et al., The Astrophysical Journal, volume 834, no. 2, January 9, 2017. * http://iopscience.iop.org/article/10.3847/1538-4357/834/2/123/meta
- AIAA SciTech Forum, Grapevine, TX, January 9-13, 2017.
 - "Computational Fluid Dynamics Analyses for the High-Lift Common Research Model Using the USM3D and FUN3D Flow Solvers," M. Rivers, C. Hunter, V. Vasta. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-0320
 - "Large-Eddy Simulation of a Compressible Mixing Layer and the Significance of Inflow Turbulence," M. Markbadi, J. DeBonis, N. Geordiadis. *
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 - "Wall-Resolved Large-Eddy Simulation of Flow Separation Over NASA Wall-Mounted Hump,"
 A. Uzun, M. Malik. *
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Papers (cont.)



- AIAA SciTech Forum (cont.)
 - "Large Eddy Simulations of High Pressure Jets: Effect of Subgrid Scale Modeling," J. Bellan,
 A. Gnanaskandan. *
 http://arc.aiaa.org/doi/abs/10.2514/6.2017-1105
 - "Advanced Modeling of Non-Equilibrium Flows Using a Maximum Entropy Quadratic Formulation," M. Priyadarshini, Y. Liu, M. Panesi. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-1612
 - "Computational and Experimental Characterization of the Mach 6 Facility Nozzle Flow for the Enhanced Injection and Mixing Project at NASA Langley Research Center," T. Drozda, et al. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-1537
 - "Relating a Jet-Surface Interaction Experiment to a Commercial Supersonic Transport Aircraft Using Numerical Simulations," V. Dippold, III, D. Friedlander. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-1853
 - "Numerical Investigation of Vibrational Relaxation Coupling with Turbulent Mixing," R. Fievet, S. Voelkel, V. Raman, P. Varghese. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-0663
 - "Optical Flow for Flight and Wind Tunnel Background Oriented Schlieren Imaging," N. Smith,
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 http://arc.aiaa.org/doi/abs/10.2514/6.2017-0472
 - "Validating a Monotonically-Integrated Large Eddy Simulation Code for Subsonic Jet Acoustics," D. Ingraham, J. Bridges. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-0456

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Papers (cont.)



- AIAA SciTech Forum (cont.)
 - "Retroreflective Background-Oriented Schlieren Imaging Results from the NASA Plume/Shock Interaction Test," N. Smith, D. Durston, J. Heineck. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-0043
 - "DPW-VI Results Using FUN3D with Focus on k-kL-MEAH2015 (k-kL) Turbulence Model,"
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- "Optimal Numerical Solvers for Transient Simulations of Ice Flow Using the Ice Sheet System Model (ISSM versions 4.2.5 and 4.11)," F. Habbal, et al., Geoscientific Model Development, vol. 10, January 10, 2017. * http://www.geosci-model-dev.net/10/155/2017/
- "Modeling of Oscillating Control Surfaces Using Overset-Grid-Based Navier-Stokes Equations Solver," G. Guruswamy, Journal of Dynamic Systems, Measurement, and Control, vol. 139, issue 3, January 10, 2017. * http://dynamicsystems.asmedigitalcollection.asme.org/article.aspx?articleid=2569565
- "Not So Lumpy After All: Modeling the Depletion of Dark Matter Subhalos by Milky Way-like Galaxies," S. Garrison-Kimmel, et al., arXiv:1701.03792 [astro-ph.GA], January 13, 2017. *
 - https://arxiv.org/abs/1701.03792

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Papers (cont.)



- "Electron Acceleration in Contracting Magnetic Islands During Solar Flares,"
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- "Particle-in-Cell Simulations of Electron and Ion Dissipation by Whistler Turbulence: Variations with Electron β," R. S. Hughes, S. P. Gary, J. Wang, The Astrophysical Journal Letters, vol. 835, no. 1, January 23, 2017. * http://iopscience.iop.org/article/10.3847/2041-8213/835/1/L15/meta
- "Numerical Investigation of the Arctic Ice-Ocean Boundary Layer and Implications for Air-Sea Gas Fluxes," A. Bigdeli, et al., Ocean Science, vol. 13, January 23, 2017. * http://www.ocean-sci.net/13/61/2017/
- "Variations of the Martian Plasma Environment During the ICME Passage on 8 March 2015—A Time-Dependent MHD Study," Y. Ma, et al., Journal of Geophysical Research: Space Physics, January 25, 2017. * http://onlinelibrary.wiley.com/doi/10.1002/2016JA023402/full
- "A Surface Density Perturbation in the TW Hydrae Disk at 95 au Traced by Molecular Emission," R. Teague, et al., The Astrophysical Journal, vol. 835, January 31, 2017. * http://iopscience.iop.org/article/10.3847/1538-4357/835/2/228

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Presentations



- AIAA SciTech Forum, Grapevine, TX, January 9-13, 2017.
 - "Contributions to the 6th AIAA CFD Drag Prediction Workshop Using Structured, Overset Grid Methods," J. Coder, H. Hue, G. Kenway, T. Pulliam, A. Sclafani. *
 http://arc.aiaa.org/doi/abs/10.2514/6.2017-0960
 - "Overset Grid Simulations for the Second AlAA Aeroelastic Prediction Workshop,"
 J. Housman, C. Kiris. *
 http://arc.aiaa.org/doi/abs/10.2514/6.2017-0640
 - "Computations of Torque-Balanced Coaxial Rotor Flows," S. Yoon, W. Chan, T. Pulliam. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-0052
 - "Nozzle Plume/Shock Interaction Sonic Boom Test Results from the NASA Ames 9- by 7-Foot Supersonic Wind Tunnel," D. Durston, S. Cliff, M. Denison, D. Dalle, et al. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-0041
 - "Computational Evaluations of Experimental Data for Sonic Boom Models with Nozzle Jet Flow Interactions," J. Jensen, M. Denison, S. Cliff. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-0042
 - "Best Practices on Overset Structured Mesh Generation for the High-Lift CRM Geometry,"
 W. Chan. *
 http://arc.aiaa.org/doi/abs/10.2514/6.2017-0362
 - "An ODE-based Wall Model for Turbulent Flow Simulations," M. Berger, M. Aftosmis. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-0528

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Presentations (cont.)



- AIAA SciTech Forum (cont.)
 - "Assessment of Wall-modeled LES Strategies Within a Discontinuous-Galerkin Spectralelement Framework," C. de Wiart, S. Murman. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-1223
 - "MiniWall Tool for Analyzing CFD and Wind Tunnel Large Data Sets," M. Schuh, et al. * http://arc.aiaa.org/doi/abs/10.2514/6.2017-1278

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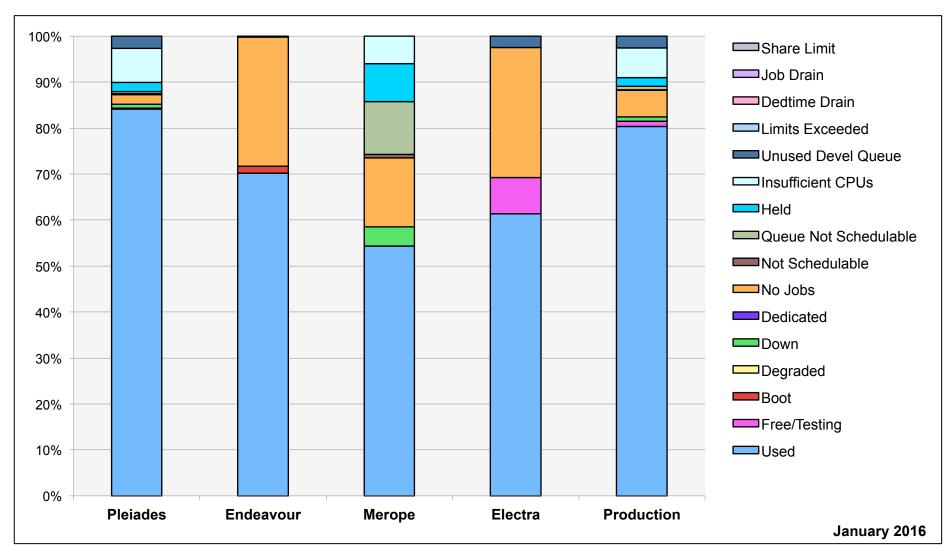
News & Events



- Exploring Drone Aerodynamics with Computers, NASA Ames Feature, January 11, 2017—Simulations of popular, commercial quadrotor drones performed by researchers on the Pleiades supercomputer show airflow interactions that offer new insights into the design of more efficient autonomous, heavy-lift, multirotor vehicles. https://www.nasa.gov/image-feature/ames/exploring-drone-aerodynamics-with-computers
 - Supercomputing Drone Aerodynamics, insideHPC, January 13, 2017.
 http://insidehpc.com/2017/01/drone-aerodynamics/
 - How drones fly: NASA releases stunning animation revealing the airflow around a quadcopter, DailyMail, January 16, 2017. http://www.dailymail.co.uk/sciencetech/article-4125220/Nasa-releases-animation-showing-airflow-drones.html
 - Watch Air Swirl Around a Quadcopter Drone's Rotors, Wired, January 24, 2017.
 https://www.wired.com/2017/01/stunning-animation-reveals-air-swirling-around-drone/
 - Have a quadcopter drone? Check out its aerodynamics, Cosmos Magazine, February 1, 2017.
 https://cosmosmagazine.com/physics/drone-aerodynamics

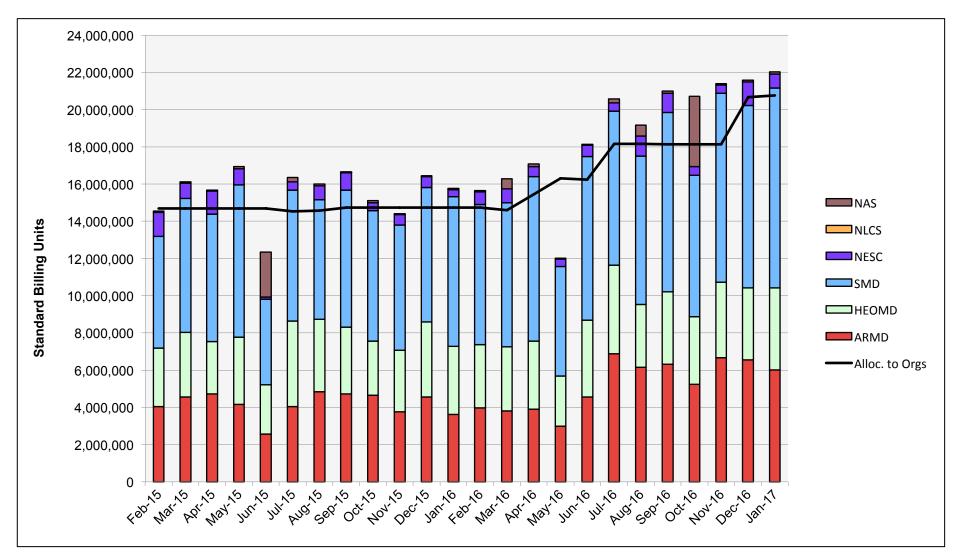
HECC Utilization





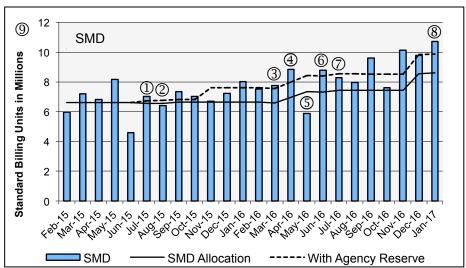
HECC Utilization Normalized to 30-Day Month

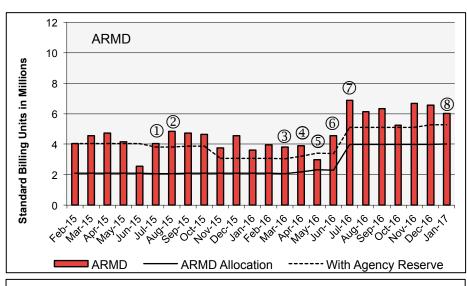


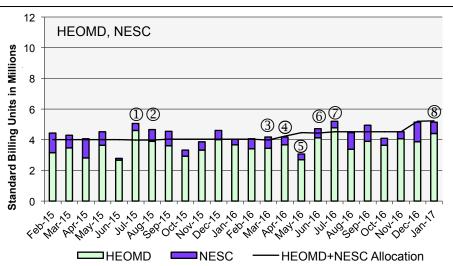


HECC Utilization Normalized to 30-Day Month





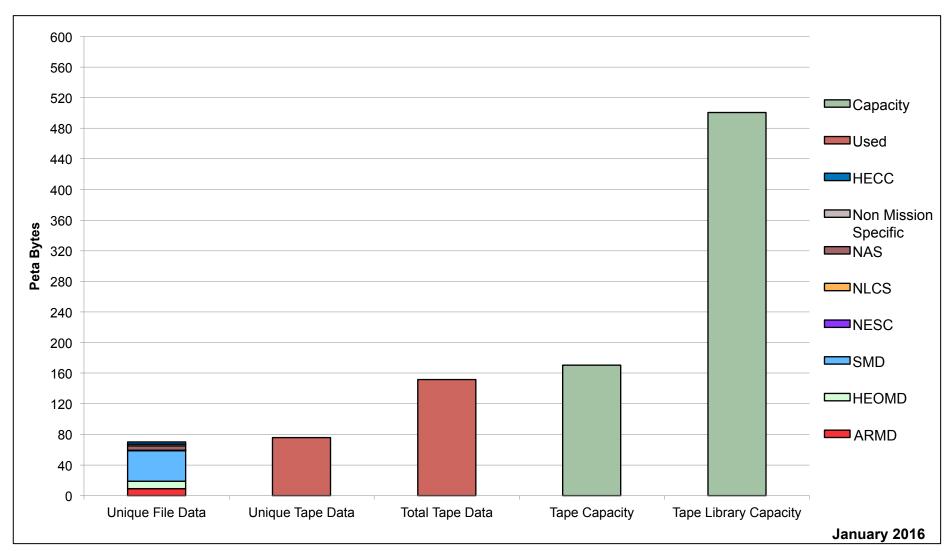




- ① 7 Nehalem ½ racks retired from Merope
- ② 7 Westmere ½ racks added to Merope
- 3 16 Westmere racks retired from Pleiades
- 4 10 Broadwell racks added to Pleiades
- S 4 Broadwell racks added to Pleiades
- © 14 (All) Westmere racks retired from Pleiades
- ② 14 Broadwell Racks added to Pleiades

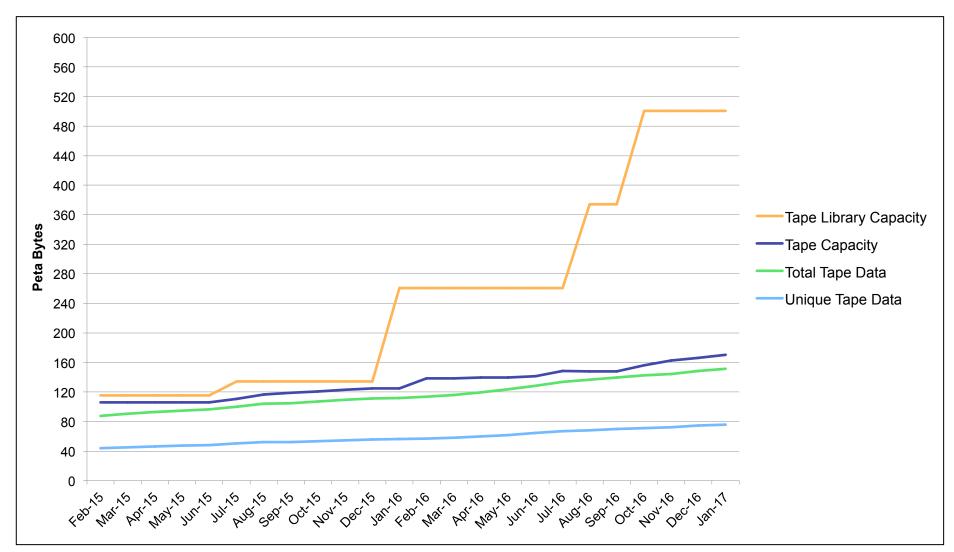
Tape Archive Status





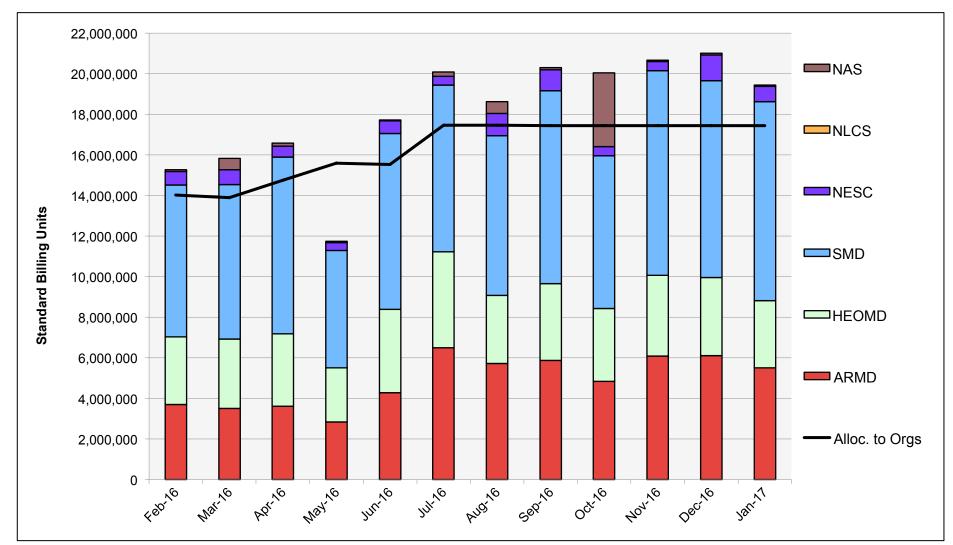
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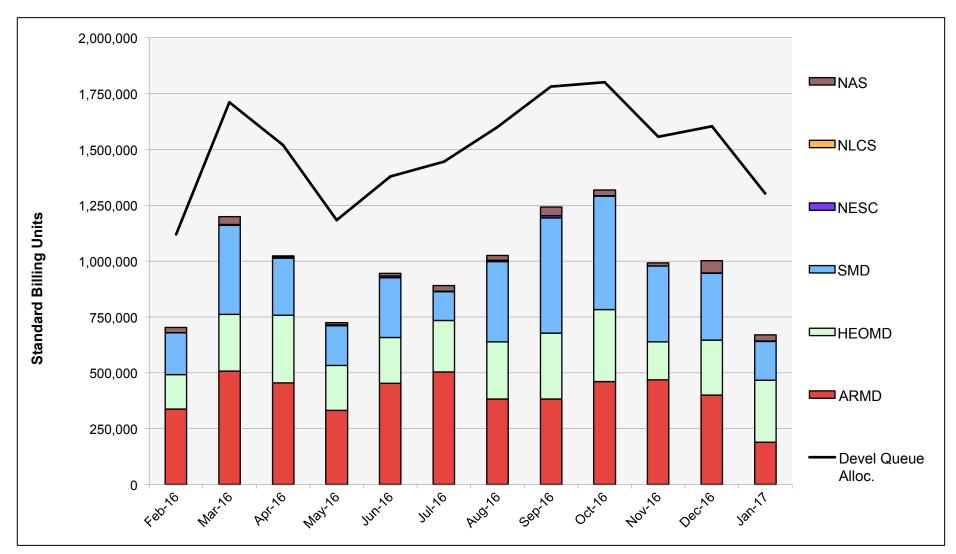
Pleiades: SBUs Reported, Normalized to 30-Day Month





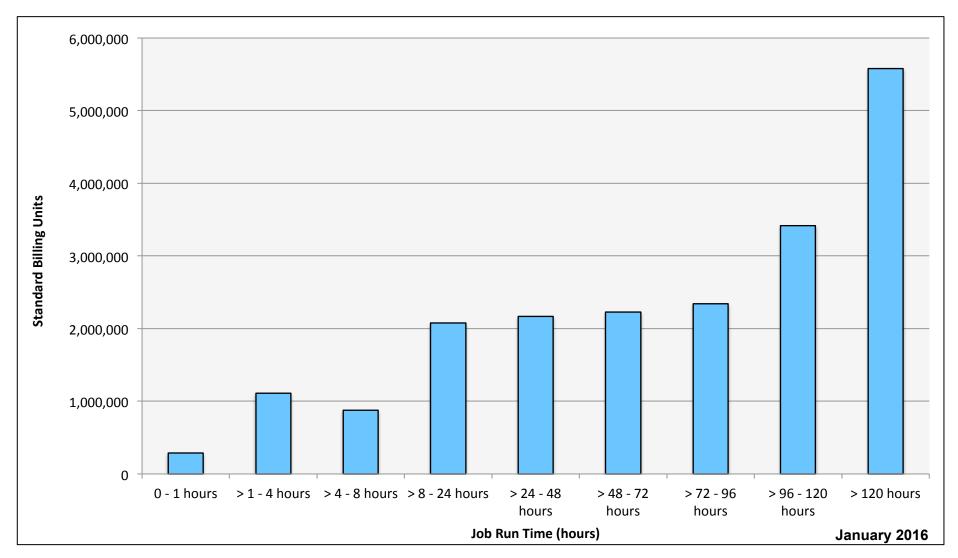
Pleiades: Devel Queue Utilization





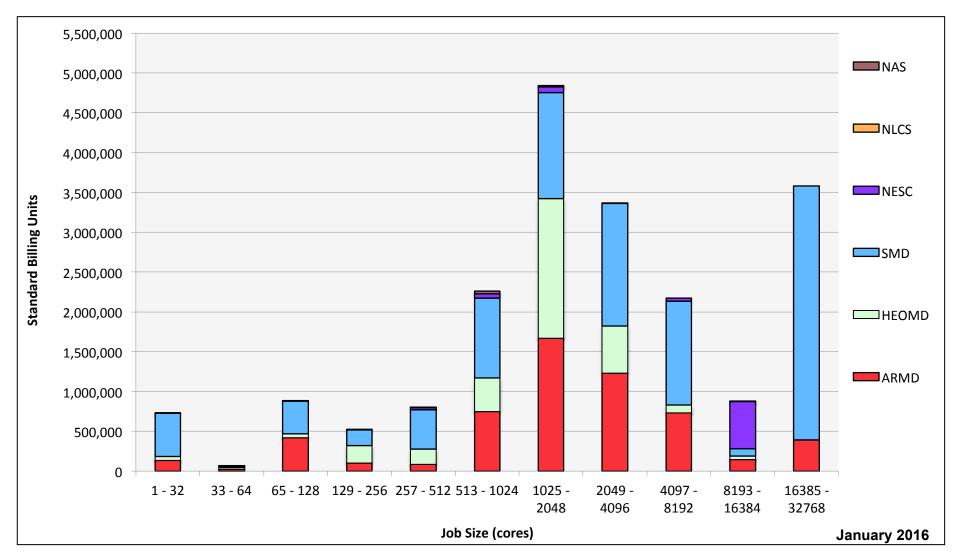
Pleiades: Monthly Utilization by Job Length





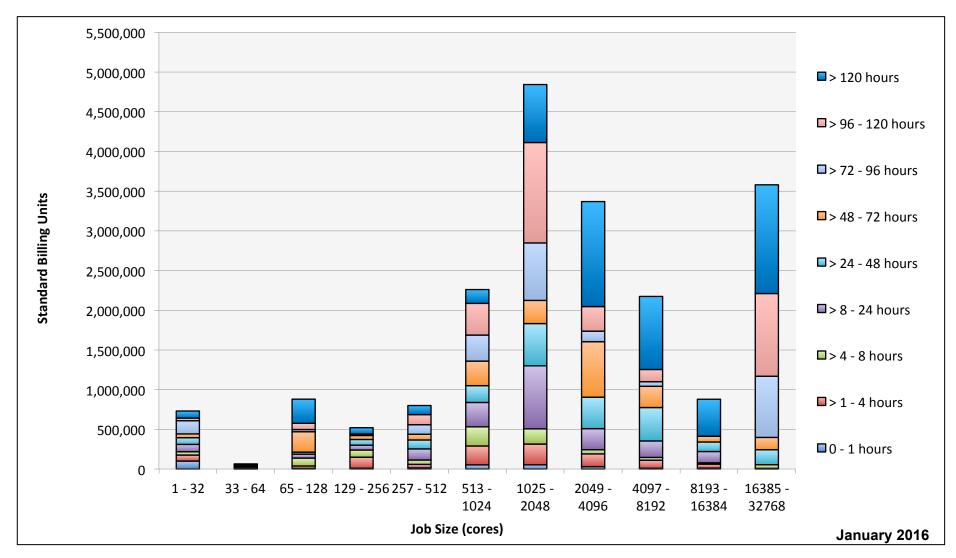
Pleiades: Monthly Utilization by Size and Mission





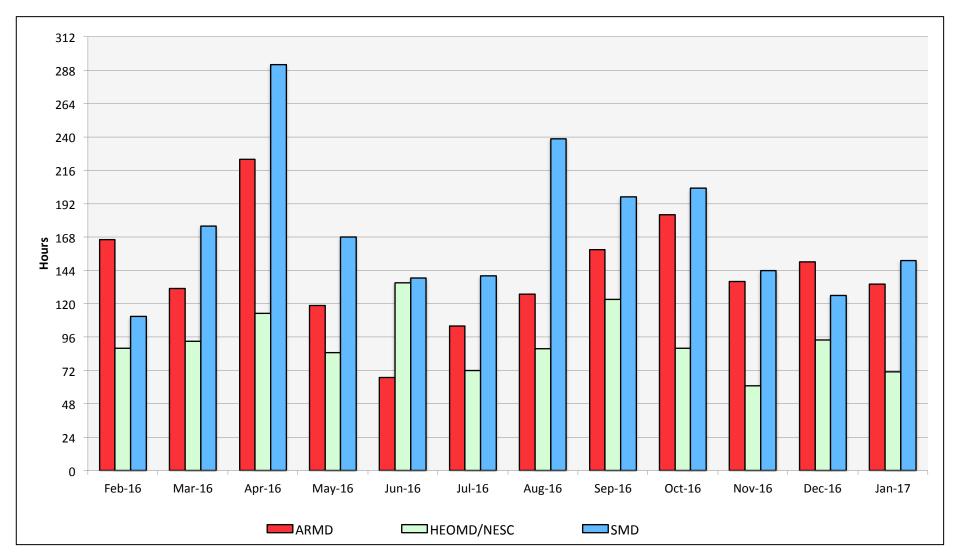
Pleiades: Monthly Utilization by Size and Length





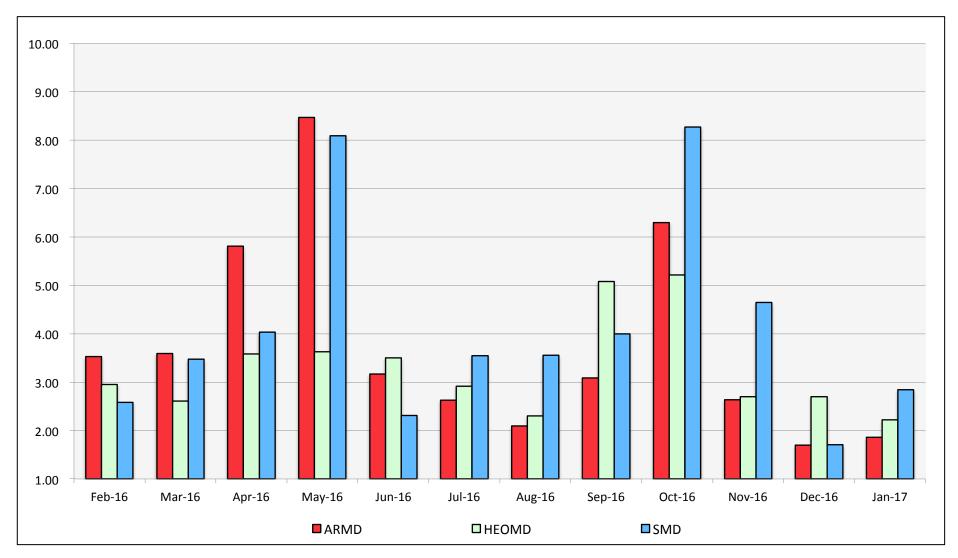
Pleiades: Average Time to Clear All Jobs





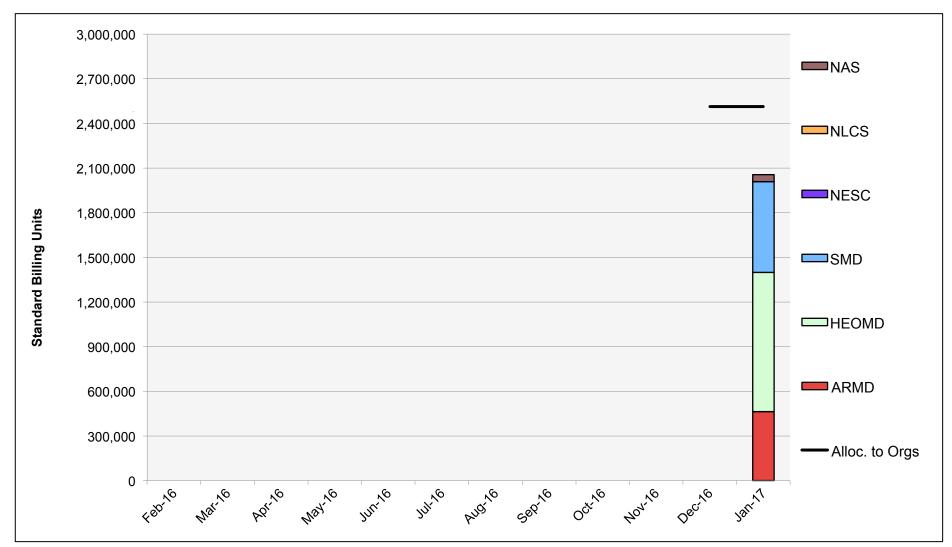
Pleiades: Average Expansion Factor





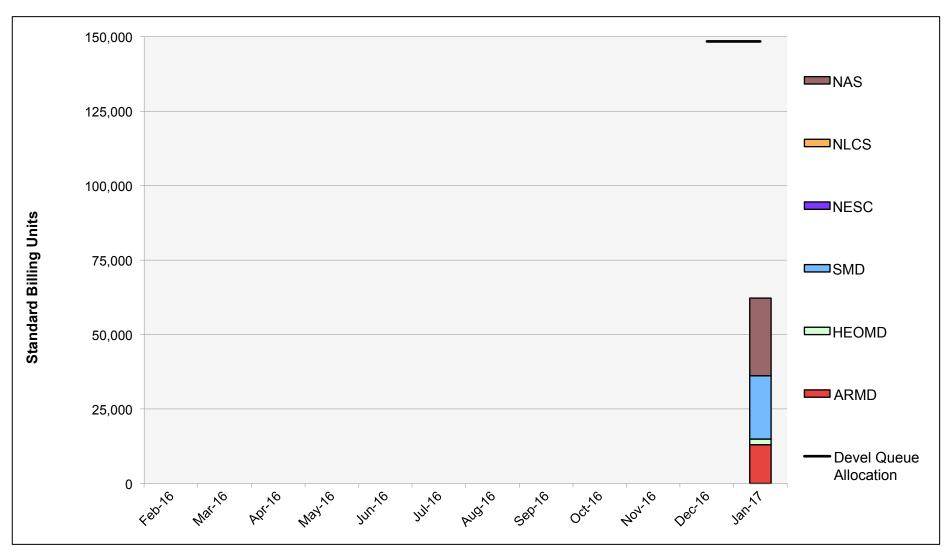
Electra: SBUs Reported, Normalized to 30-Day Month





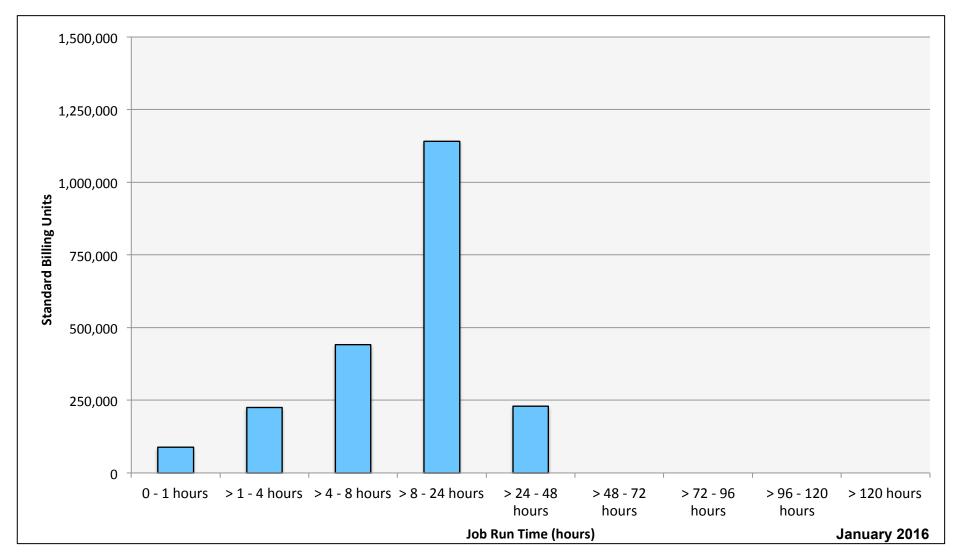
Electra: Devel Queue Utilization





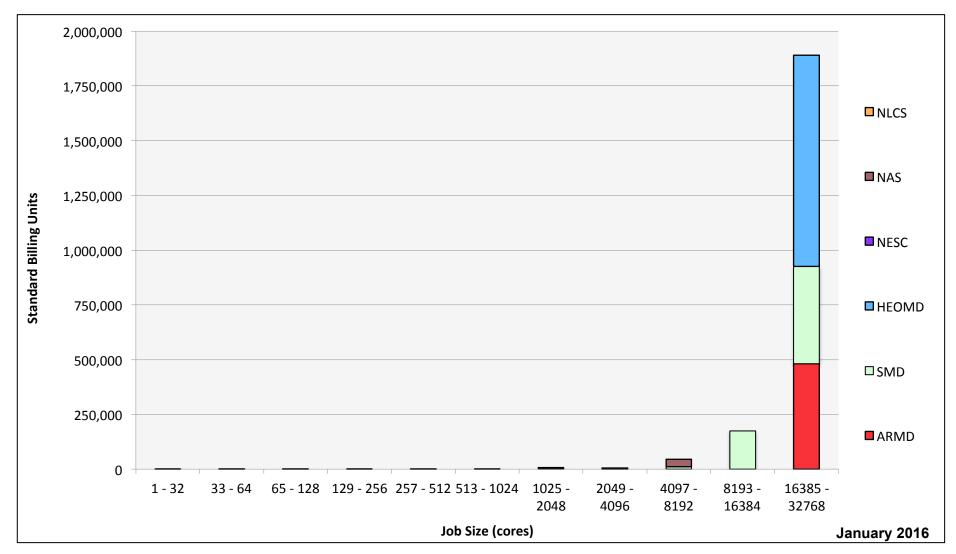
Electra: Monthly Utilization by Job Length





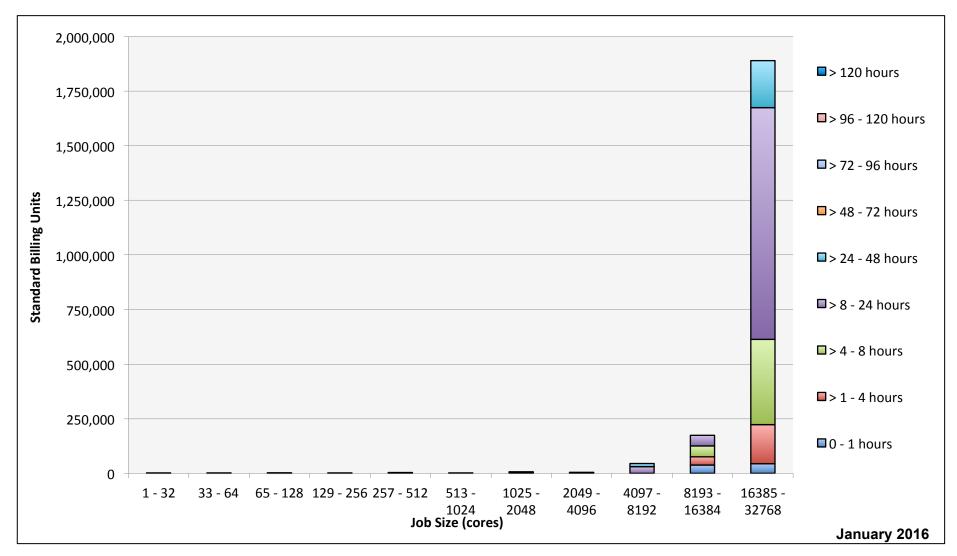
Electra: Monthly Utilization by Size and Mission





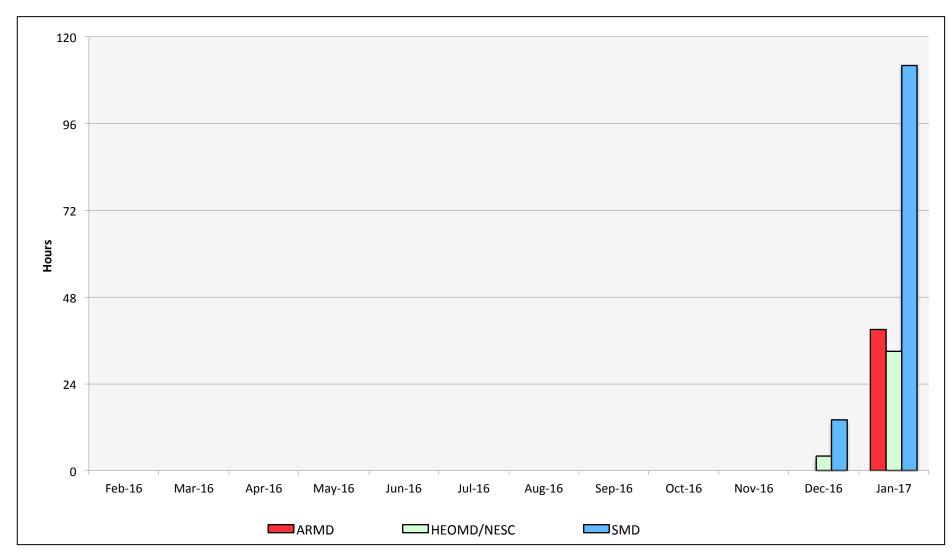
Electra: Monthly Utilization by Size and Length





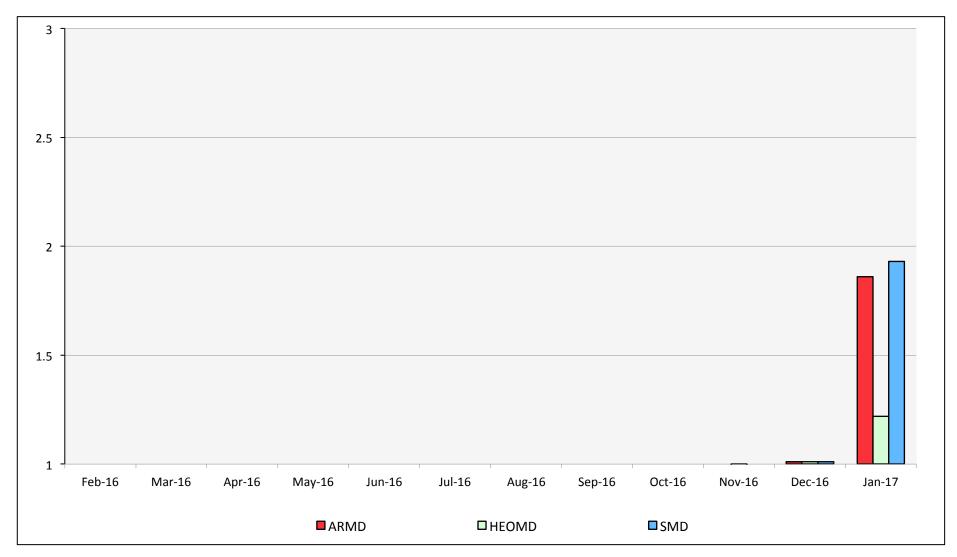
Electra: Average Time to Clear All Jobs





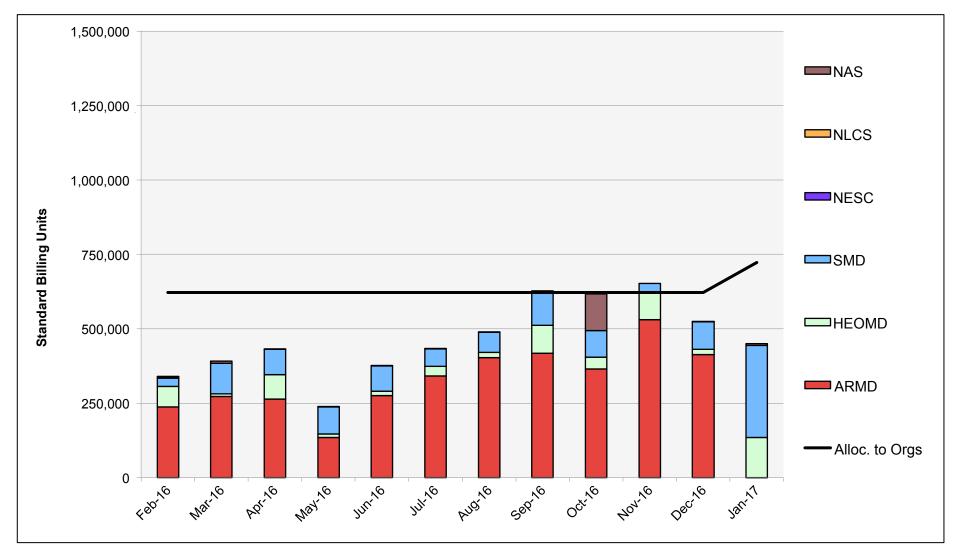
Electra: Average Expansion Factor





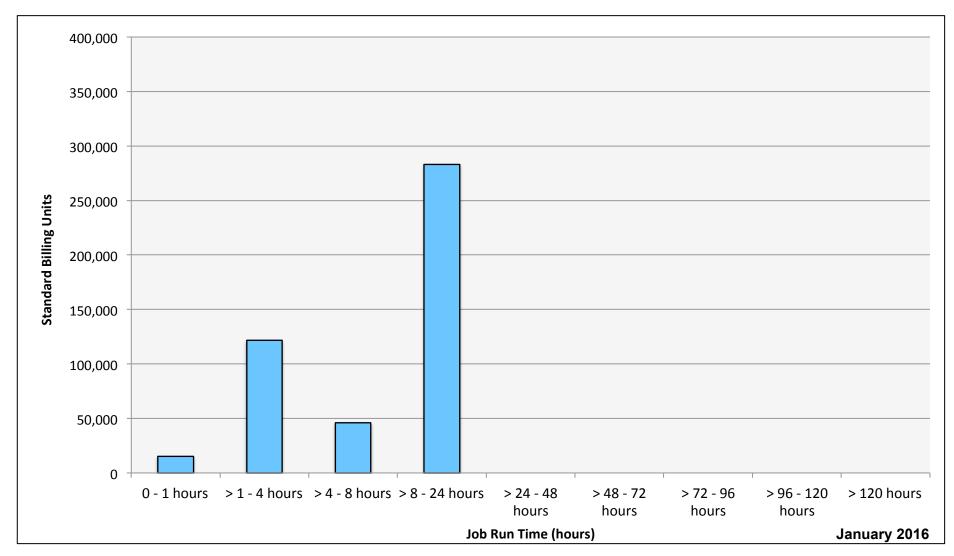
Merope: SBUs Reported, Normalized to 30-Day Month





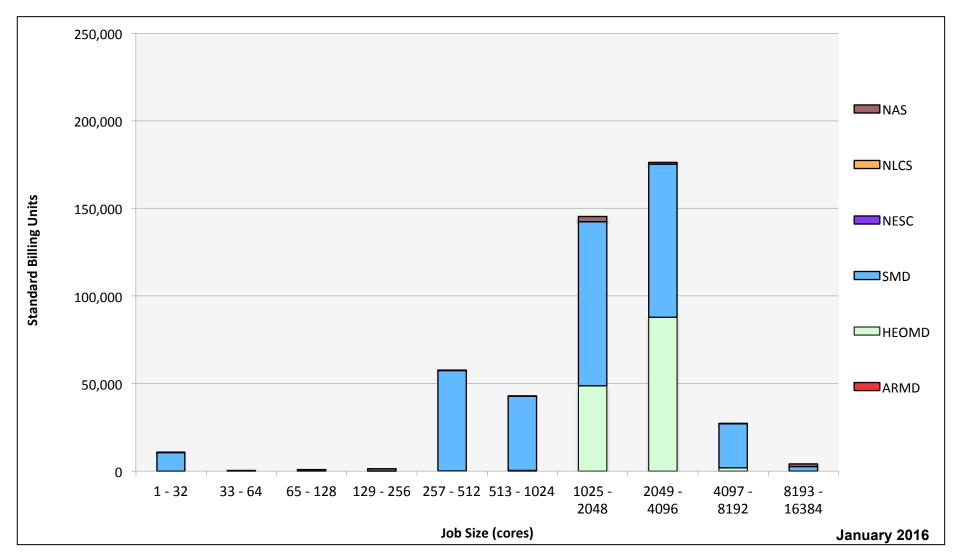
Merope: Monthly Utilization by Job Length





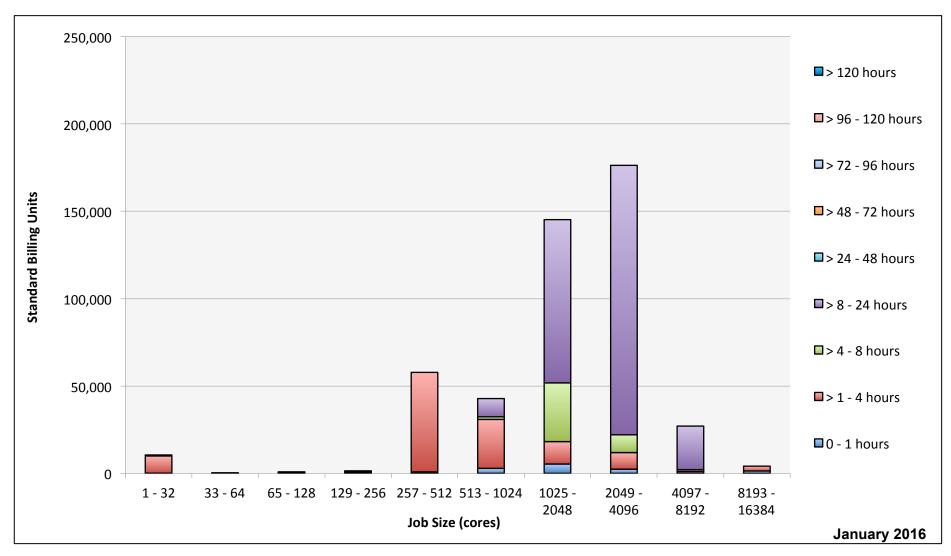
Merope: Monthly Utilization by Size and Mission





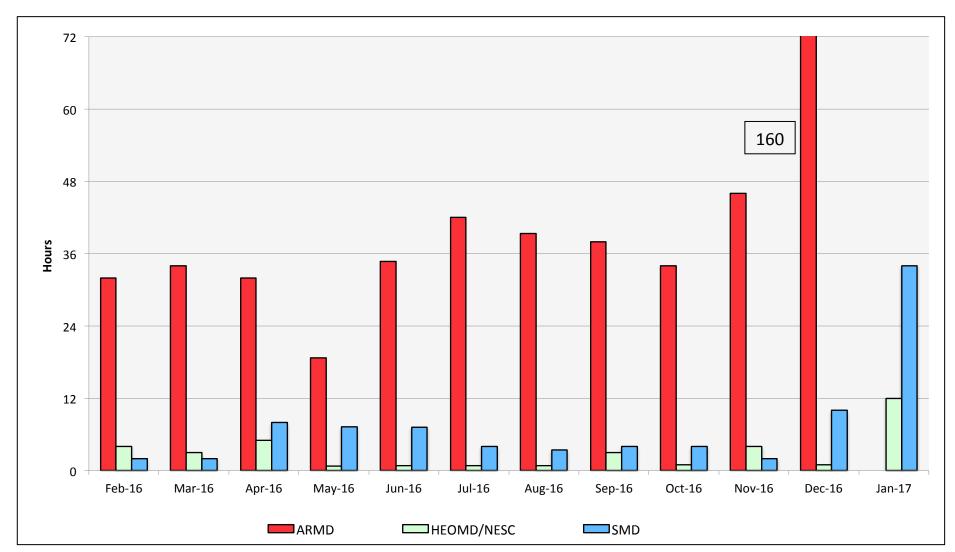
Merope: Monthly Utilization by Size and Length





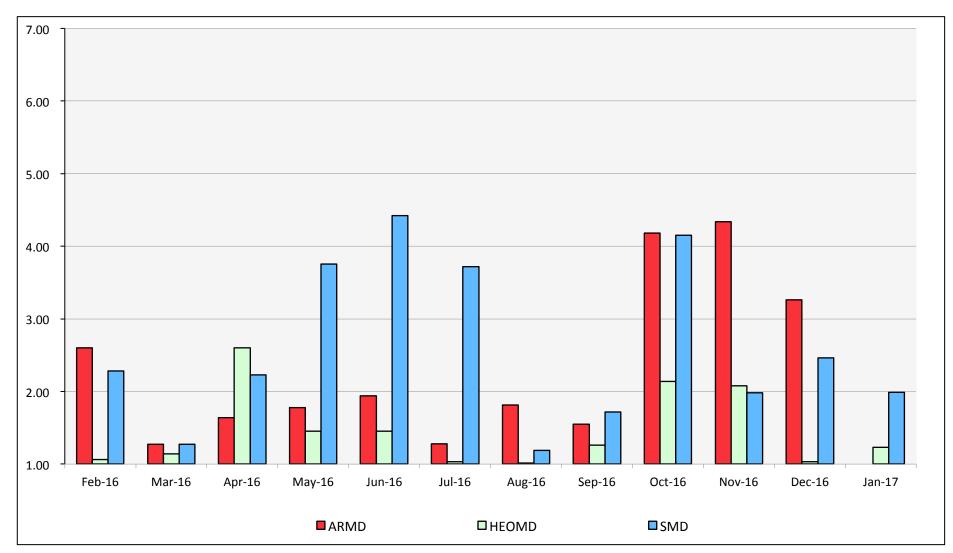
Merope: Average Time to Clear All Jobs





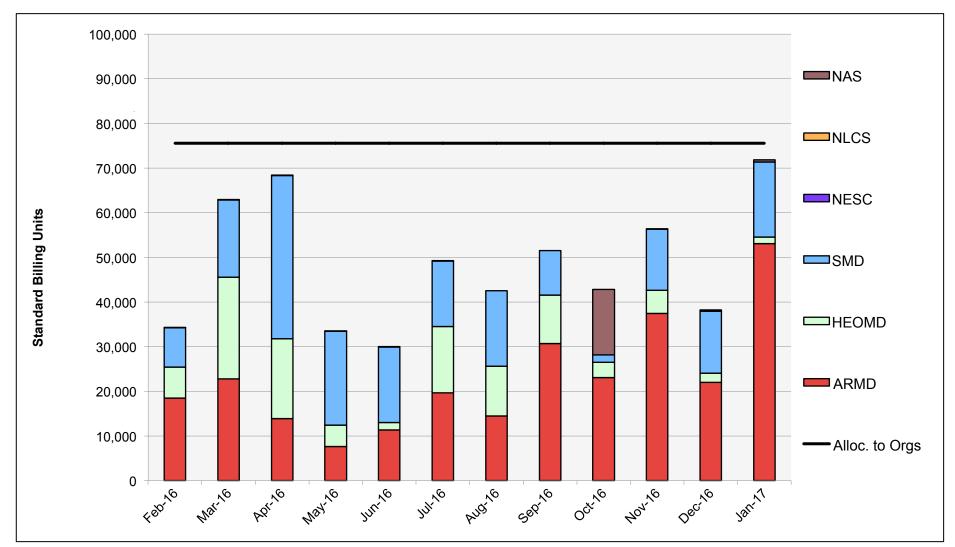
Merope: Average Expansion Factor





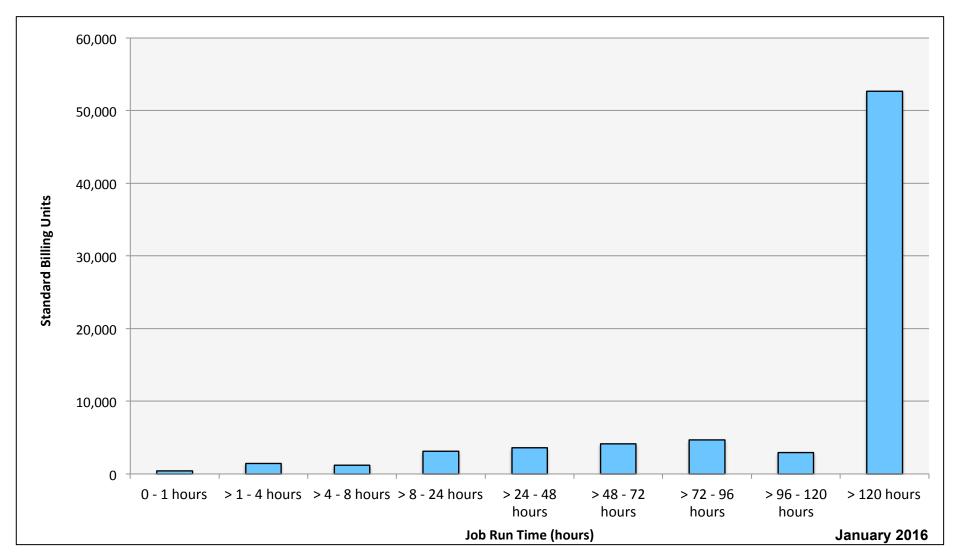
Endeavour: SBUs Reported, Normalized to 30-Day Month





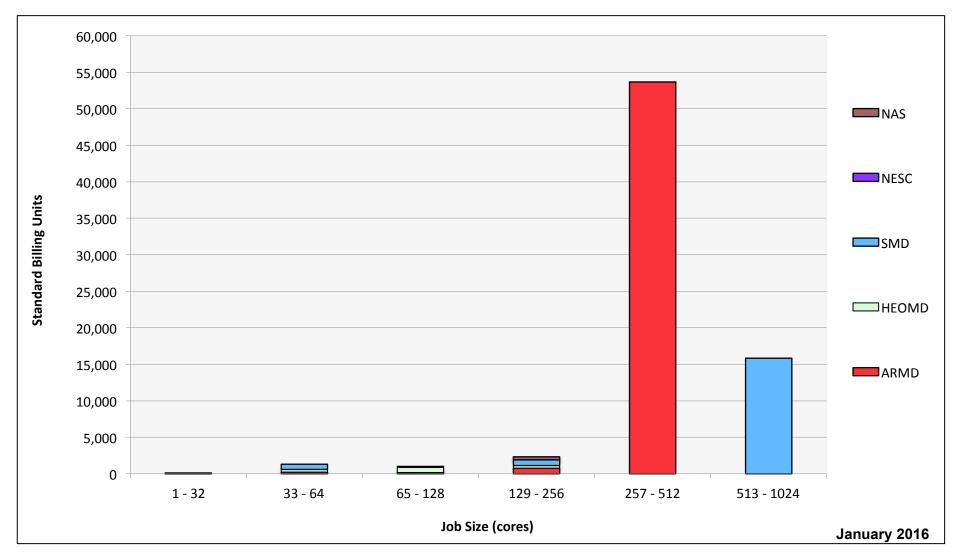
Endeavour: Monthly Utilization by Job Length





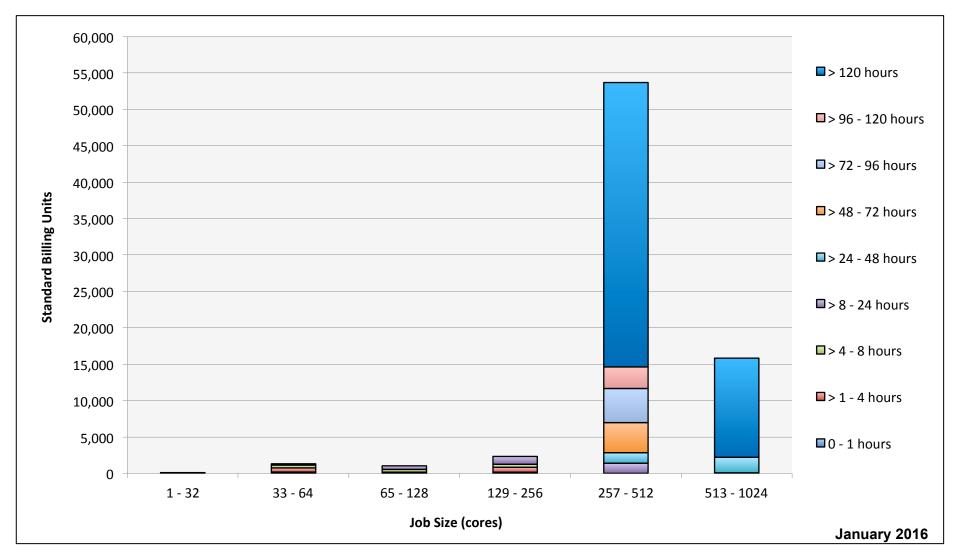
Endeavour: Monthly Utilization by Size and Mission





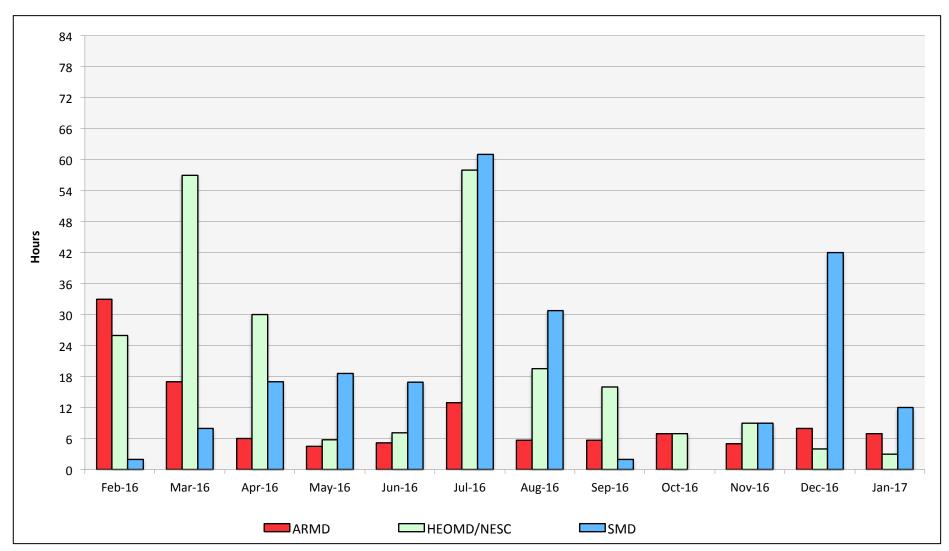
Endeavour: Monthly Utilization by Size and Length





Endeavour: Average Time to Clear All Jobs





Endeavour: Average Expansion Factor



